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L7 ANSWER 1 OF 1 WPIDS COPYRIGHT 2005 THE THOMSON CORP on STN  
 ACCESSION NUMBER: 2002-382419 [41] WPIDS  
 DOC. NO. CPI: C2002-107712  
 TITLE: Mono- or poly-quaternary polysiloxane for use e.g. in cosmetics, polish and detergent formulations, contains two siloxane units attached to a central secondary or tertiary amino or quaternary ammonium structure.  
 DERWENT CLASS: A26 A82 A96 A97 D21 D25 F06 G02  
 INVENTOR(S): FIRSTENBERG, D; KROPGANS, M; LANGE, H; SOCKEL, K; STACHULLA, K; TEUBER, S; WAGNER, R; WITOSSEK, A  
 PATENT ASSIGNEE(S): (GENE) GE BAYER SILICONES GMBH & CO KG  
 COUNTRY COUNT: 97  
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 2002010256	A1	20020207	(200241)*	GE	48	C08G077-46	--
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ							
NL OA PT SD SE SL SZ TR TZ UG ZW							
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK							
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR							
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU							
SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW							
AU 2001091686	A	20020213	(200242)			C08G077-46	
EP 1309648	A1	20030514	(200333)	GE		C08G077-46	
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT							
RO SE SI TR							
JP 2004521967	W	20040722	(200448)		80	C08G077-54	

## APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2002010256	A1	WO 2001-EP8698	20010727
AU 2001091686	A	AU 2001-91686	20010727
EP 1309648	A1	EP 2001-971791	20010727
		WO 2001-EP8698	20010727
JP 2004521967	W	WO 2001-EP8698	20010727
		JP 2002-515983	20010727

## FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2001091686	A Based on	WO 2002010256
EP 1309648	A1 Based on	WO 2002010256
JP 2004521967	W Based on	WO 2002010256

PRIORITY APPLN. INFO: DE 2000-10036524 20000727

## INT. PATENT CLASSIF.:

MAIN: C08G077-46; C08G077-54  
 SECONDARY: A61K007-075; A61K007-08; A61K007-11; A61K007-48;  
 C07F007-10; D06M015-643; D06M015-647

## BASIC ABSTRACT:

WO 200210256 A UPAB: 20020701

NOVELTY - Mono- or poly-quaternary polysiloxanes with two siloxane units attached to a secondary or tertiary amino or quaternary ammonium structure by alkylation of the amino nitrogen atoms with suitably functionalized siloxane compounds.

DETAILED DESCRIPTION - Mono- or poly-quaternary polysiloxanes of formula (I).

S-K-Q1-K-S (I)

S = a group of formula  $(R1)_3Si-(OSi(R1)_2)_n-O-Si(R1)-O-Si(R1)_3$  or  $(R1)_3-(O-Si(R1)_2)_n-O-Si(R1)_2-$ ;

R1 = 1-22C (fluoro)alkyl, or aryl;

n = 0-1000;

Q1 = a secondary or tertiary amine or quaternary ammonium structure (-NH-, -NR2- or -NR2R3+-);

R2 = mono- or di-valent, linear, branched or cyclic 1-30C hydrocarbon residue (optionally interrupted by O, NH, CO or CS or substituted with OH), or a single bond to group K;

R3 = monovalent 1-30C hydrocarbyl (optionally modified as for R2) or a structure -A-E-;

A = -CH2COO-, -(CH2)2COO- or -(CH2)3COO-;

E = a polyalkylene oxide unit of formula  $-(CH2CH2O)_q-(CH2CH(CH3)O)_r-$  R4;

q = 1-200;

r = 0-200;

R4 = H or 1-20C hydrocarbyl (linear, branched, cyclic, optionally acetylenic, olefinic or aromatic, optionally with -O- or -CO- groups or substituted with OH);

K = a di- or tri-valent 2-40C hydrocarbon group (linear, cyclic or branched, optionally interrupted by -O-, -NH-, -NR1-, -N=, -CO- or -CS- and/or substituted with OH) or a group Q2;

Q2 = -NH-, -NR5- or -NR5R3+-; and

R5 = a mono- or di-valent 1-20C hydrocarbon residue (optionally modified as for R2), possibly with the free valency attached to Q1

INDEPENDENT CLAIMS are also included for:

(a) a method for the production of (I) in which Q1 = -NR2R3+-, by alkylating tertiary amino group-containing monofunctional siloxane derivatives with reactive monofunctional siloxane derivatives obtained by hydrosilylation, e.g. of halo-alkenes, unsaturated halocarboxylic acid esters or epoxy-functional alkenes, with monofunctional Si-H compounds of formula (S)-H, using a mol ratio of (tertiary amino functions):(reactive alkylating groups) = (100:1)-(1:1);

(b) a method for the production of (I) in which Q1 = -NR2-, by direct hydrosilylation of unsaturated compounds containing sec. amino groups with monofunctional Si-H siloxanes, followed by reaction with monofunctional alkylating siloxane intermediates (MFS) to form the tertiary amino groups, using a (secondary amine):(alkylating siloxane) ratio of 1:1;

(c) an alternative method to (b) in which di-sec. amines (preferably piperazine) are converted into tertiary amino compounds by reaction with MFS in a mol ratio of 1:2;

(d) a method for the production of (I) with equimolar amounts of tert. amino and quaternary ammonium functions by reaction of secondary-tertiary diamines (preferably N-methylpiperazine) with MFS (preferably epoxide derivatives) in a mol. ratio of 1:1 to give a di-tertiary aminosiloxane, followed by further reaction with 1 mol MFS.

USE - In cosmetic formulation for skin- and hair-care, in polishes for hard surfaces, in formulations for drying cars and other hard surfaces after washing, for the finishing of textiles and textile fibres, as separate softeners after washing textiles with non-ionic or anionic/non-ionic detergents and as softeners in textile washing

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formulations based on such detergents, where the amino groups may be in the form of amine or amine salt depending on the pH (claimed).

ADVANTAGE - Mono- or poly-quaternary polysiloxanes without the disadvantages of prior-art systems, comprising two independently mobile siloxane units linked by an amino or ammonium element. The use of these compounds in cosmetic hair preparations (for example) gives good results with regard to strengthening, shine, hold, body, volume, moisture regulation, color retention, protection (from UV, salt water etc.), reshapeability, antistatic properties and colorability etc.

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TECHNOLOGY FOCUS:

WO 200210256 A1UPTX: 20020701

TECHNOLOGY FOCUS - POLYMERS - Preferred Methods: Compounds (I) with tertiary amino and quaternary ammonium groups are obtained by reaction of di-secondary amines (preferably piperazine) with 2 moles MFS, followed by alkylation with epoxides in presence of acids, alkyl halides or halo-acid esters, preferably halocarboxylates of alkylene oxides, using a mol ratio of (tert. amino groups):(alkylating agent) = (100:1)-(1:1); alternatively, sec. amines (preferably dimethylamine) or sec.-tert. diamines (preferably N-methyl-piperazine) are reacted with MFS (preferably epoxy derivatives) in 1:1 mol ratio to give compounds with tert. or di-tert. aminosiloxane structures which are then reacted with a difunctional alkylating agent (preferably in 2:1 mol ratio) to give siloxanes with quaternary ammonium groups, with or without tert. amino groups. Preferred halocarboxylate esters are based on low-mol. wt., oligomeric or polymeric alkylene oxides of formula HO-E (see above), preferably mono-substituted derivatives of di-, tri-, tetra- or oligo-ethylene glycols with molecular weights of 300-1000, or dipropylene glycol, especially oligo-ethylene glycols with molecular weights of 400, 600 or 800.

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Reagents: Preferred starting materials for the production of MFS (by hydrosilylation) comprise allyl chloride or bromide, allyl chloroacetate or chloropropionate, propargyl chloroacetate or 3-chloropropionate, vinylcyclohexene oxide and allyl glycidyl ether. Preferred sec. amines for direct hydrosilylation (method b above) are N-methylallylamine or an amine of formula  $H_2C=CHCH_2OCH_2CH(OH)CH_2NHCH_3$ .

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB

MANUAL CODES: CPI: A05-H01A; A06-A00B; A06-A00D; A10-E01; A10-E03;  
D08-B10; F03-C05; F03-J03; G02-A05; G02-C

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